T-12
Theoretical Chemistry & Molecular Physics

Collaborating with the Semiconductor Industry

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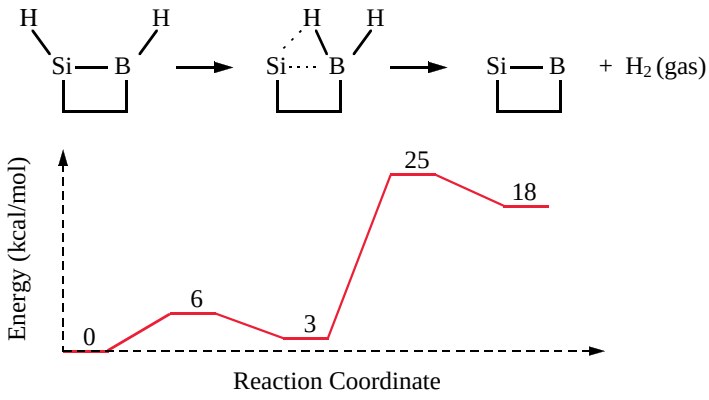
For several years, members of the Theoretical Chemistry & Molecular Physics Group (T-12) at Los Alamos have engaged in research projects with industrial collaborators in the semiconductor industry. Supported under DOE Cooperative Research and Development Agreements (CRADA), these projects may receive funding from a variety of sources.

High Pressure Oxidation of Silicon Wafers

The first of these projects began in 1993, pairing Los Alamos researchers with scientists from GaSonics, Inc., and Texas Instruments. GaSonics is an equipment manufacturing concern in California, which sought to enlist the modeling and simulation capabilities of the Laboratory in guiding the design of a next-generation single-wafer device for growing oxide films on silicon wafers. Using high pressure water under supercritical conditions, gate-quality oxide films can be grown in a few minutes. To be commercially viable, the process needs to generate films of uniform thickness across the wafer, and films that are free from particulate contamination.

Si-B (100) Dimer (Si_8BH_{14} Cluster Model)



The GaSonics high pressure oxidation device consisted of a fragile internal reaction chamber made entirely of quartz. Under supercritical conditions, silica is quite soluble in steam. The Los Alamos modeling effort, led by Shirish Chitanvis and David Hanson (T-12), focused on development of software capable of modeling the actual flow patterns in the GaSonics reaction chamber and in the silica boiler upstream of the chamber. The modeling software needed to be able to track temperature and pressure changes throughout the system, and model the effects of these changes on the dissolution and nucleation kinetics of quartz.

As a result of this joint research effort, Los Alamos scientists were able to provide valuable guidance to the industrial collaborators in refining the design of the reaction chamber and of the upstream boiler. The importance of eliminating cold zones (where nucleation of particulates could initiate) was identified. The Los Alamos scientists benefitted by significantly improving their modeling capabilities in flow chemistry in the presence of nucleation physics. Spinoffs of this research led to other projects in modeling the arterial flow of blood, and in modeling the cleaning of surfaces using supercritical carbon dioxide.

The Center for Semiconductor Modeling and Simulation

More recently, Los Alamos scientists from many groups in T Division have joined efforts to work with the Semiconductor Research Corporation in developing modeling and simulation capabilities of interest to the manufacture of semiconductor devices. In a large effort coordinated by David C. Cartwright, this project encompasses work not only at Los Alamos, but also at Lawrence Livermore National Laboratory and at Sandia National Laboratories.

Work in the T-12 Group on this project has focused on the modeling of the topography of patterned wafers. In manufacturing semiconductor devices, the silicon wafer undergoes many processing phases, which alternately deposit onto the surface thin films of materials, or etch away materials from the surface of the wafer. The resulting patterned wafer may have a quite complicated topography, and the industry needs to be able to accurately predict both the three-dimensional geometry of the wafer and its physical and chemical properties.

Accurate modeling of the deposition or etching of materials on a silicon wafer requires a detailed picture of the surface chemistry which takes place there. One of these projects in T-12, to model the etching of chlorine, has been described in another feature article. Here we mention another calculation, led by Jeff Hay (T-12), who has studied the effect of chemical vapor codeposition of silicon and boron onto silicon surfaces. To produce a region on a wafer that has been doped with the element boron, the standard process has been to accelerate ions of boron into a silicon surface. This high energy implantation process has the undesirable side effect of damaging the silicon surface so that it must later be annealed. The alternative method we have been studying would grow a layer of silicon and boron (in the right amount) simultaneously. Experiments have shown that the growth rate of deposited silicon (layer thickness vs. time) is actually faster when there is some boron dopant present in the reacting gas than when the boron is absent.

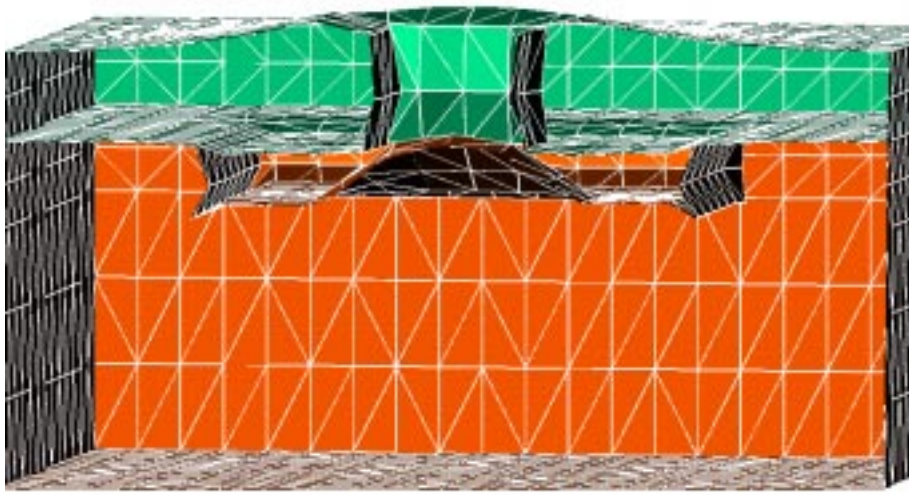


Figure 2

Quantum chemistry calculations provide an understanding of this observed result. Normally, the rate-limiting step for silicon growth from silane gas (Si2H6) is the recombination (and subsequent desorption) of hydrogen gas on the newly-formed silicon surface. When there are boron atoms exposed on the surface, this same all-important recombination step can take place above the boron atom with much less energy required. Our calculations show that recombination above a Si-Si dimer site requires 79 kcal/mol of energy, but above a Si-B dimer site (Figure 1), only 25 kcal/mol are required. The rate of a recombination reaction is proportional to exp(-E/kT), where E is the energy requirement, T is the temperature, and k is Boltzmann's constant. Therefore, these calculations are consistent with the faster growth rate for the doped film, because the energy requirement for recombination is lower.

The results of these detailed investigations into surface chemistry mechanisms is then fed to a second topography effort to model the time evolution of film profiles on wafers during the processing phase. This software development effort is a customer of the three-dimensional grid generation effort (X3D) being coordinated from the T-1 Group by Denise George. The accurate tracking of the evolution of material interfaces requires a robust adaptive meshing capability, because the evolving interfaces change their topography and topology in complicated ways during a processing step. The principal thin film software development effort in T-12 is embodied in the code "TopoSim3D." This code follows the three-dimensional evolution of material interfaces with time, based on a solid geometry model of the initial wafer state, the physics of transport of materials to the wafer surface, and of the reaction chemistry of materials at the surface. Figure 2 shows an example calculation of the deposition of material onto a wafer containing an overhang structure, resembling a skylight in the roof of a house. Test structures of this type are manufactured by industry specifically to assist modeling efforts in discriminating mechanisms of material transport to surfaces. When the pressure is low enough, material will be deposited on the underside of the overhang only if there are multiple reflections or re-emission of materials from other surfaces which are in the direct line-of-sight of the deposition source.

The variety of interesting scientific problems which characterize research in the semiconductor industry makes this effort very beneficial to modeling and simulation capabilities at Los Alamos. Existing modeling capabilities are strongly enhanced by applying existing tools to new problems, especially when these new scientific challenges require the development of newer, broader, and more robust algorithms for applying a molecular level understanding of forces to obtain a macroscopic understanding of the properties of materials.

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